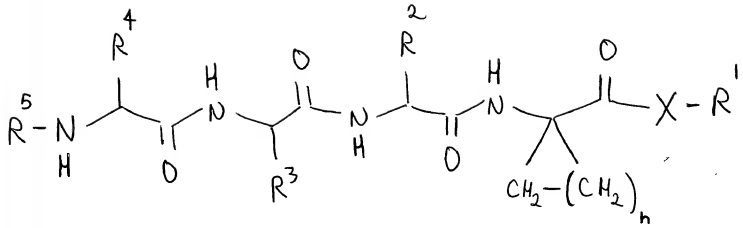
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O
R3
O
CH2-(CH2)n

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=> fil reg; d stat que l4

FILE 'REGISTRY' ENTERED AT 12:03:16 ON 17 FEB 2000
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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 13, 1999

  Please note that search-term pricing does apply when
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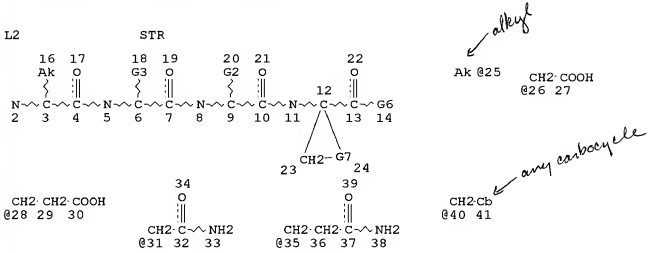
L2 STR

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DEFAULT ECLEVEL IS LIMITED
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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
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SEARCH TIME: 00.00.01


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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
                    Searched by Barb O'Bryen, STIC  308-4291
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carbocycle at 41 is monocyclic, unsaturated & has exactly 6 carbons

FILE COVERS 1967 - 17 Feb 2000 VOL 132 ISS 8
FILE LAST UPDATED: 16 Feb 2000 (20000216/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REGlstRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

L2 STR
L4 32 SEA FILE=REGISTRY SSS FUL L2
L5 8 SEA FILE=CAPLUS ABB=ON L4

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L5 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1999:682201 CAPLUS
DOCUMENT NUMBER: 132:78839
TITLE: Long-range electron transfer in rigid 310-helical oligopeptides containing redox cyclic .alpha.-amino acids
AUTHOR(S): Lang, Kamil; Kuki, Atsuo
CORPORATE SOURCE: Department of Chemistry, University of California, Santa Cruz, CA, USA
SOURCE: Photochem. Photobiol. (1999), 70(4), 579-584
CODEN: PHCBAP; ISSN: 0031-8655
PUBLISHER: American Society for Photobiology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Intrahelical photoinduced electron transfer processes (ET) in conformationally restricted oligopeptides have been studied by nanosecond time-resolved transient spectroscopy. The helical peptides were constructed from sterically hindered .alpha.-aminoisobutyric acid (Aib) and two cyclic .alpha.-amino acids (Aib class) bearing electron acceptor and donor side chains (DkNap, ThQx). This helical backbone design provides high conformation stability, as previously demonstrated, and yields reliable 310-helical architectures in soln. The forward ET between ThQx and 3DkNap is followed by a slow back ET thus giving rise to an accumulation of the charge-sepd. ion pairs for hundreds of nanoseconds. We demonstrate the modulation of electronic interactions by the no. of intervening Aib residues sepg. acceptor-donor side chains and propose modifications of the peptide framework by inclusion of a non-Aib amino acid residue. These well-defined and sterically stable frameworks are suited for the precise evaluation of intrahelical electron transfer processes mediated by peptides.

IT **253670-46-1P 253670-47-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of in the synthesis of rigid 310-helical oligopeptides contg. redox cyclic .alpha.-amino acids for study of

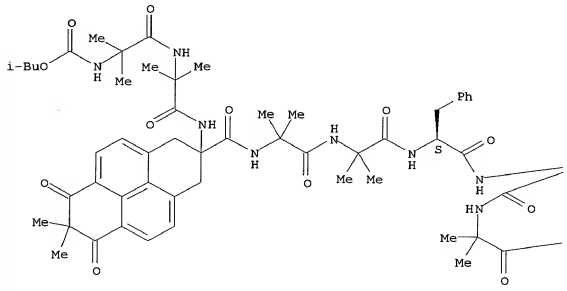
long-range electron transfer)

RN 253670-46-1 CAPLUS

CN .beta.-Alanine, 2-methyl-N-[(2-methylpropoxy)carbonyl]alanyl-2-methylalanyl-2-amino-1,2,3,6,7,8-hexahydro-7,7-dimethyl-6,8-dioxo-2-pyrenecarbonyl-2-methylalanyl-2-methylalanyl-L-phenylalanyl-7-amino-7,8-dihydro-6H-cyclopenta[g]quinoxaline-7-carbonyl-2-methylalanyl-2-methylalanyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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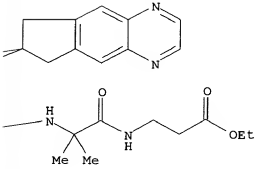
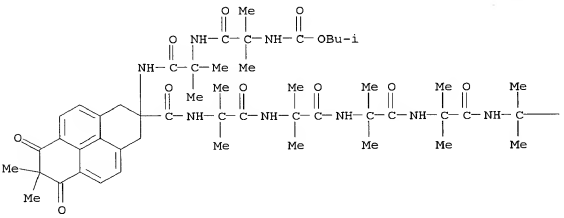


RN 253670-47-2 CAPLUS

CN .beta.-Alanine, 2-methyl-N-[(2-methylpropoxy)carbonyl]alanyl-2-methylalanyl-2-amino-1,2,3,6,7,8-hexahydro-7,7-dimethyl-6,8-dioxo-2-

pyrenecarbonyl-2-methylalanyl-2-methylalanyl-2-methylalanyl-2-methylalanyl-2-methylalanyl-7-amino-7,8-dihydro-6H-cyclopenta[g]quinoxaline-7-carbonyl-2-methylalanyl-2-methylalanyl-, ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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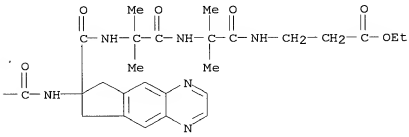


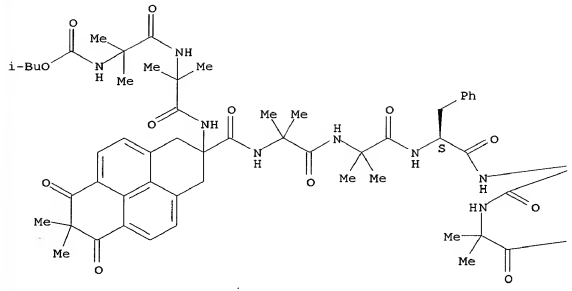
IT **253670-48-3P 253670-49-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of as rigid 310-helical oligopeptides contg. redox cyclic .alpha.-amino acids for study of long-range electron transfer)

RN 253670-48-3 CAPLUS

CN .beta.-Alanine, 2-methyl-N-[(2-methylpropoxy)carbonyl]alanyl-2-methylalanyl-2-amino-1,2,3,6,7,8-hexahydro-7,7-dimethyl-6,8-dioxo-2-pyrenecarbonyl-2-methylalanyl-2-methylalanyl-L-phenylalanyl-7-amino-2,3,4,6,7,8-hexahydro-1,4-dimethyl-1H-cyclopenta[g]quinoxaline-7-carbonyl-2-methylalanyl-2-methylalanyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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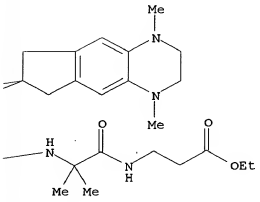
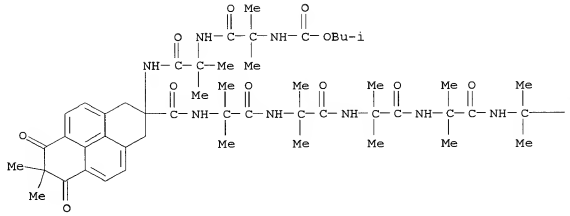


RN 253670-49-4 CAPLUS
CN .beta.-Alanine, 2-methyl-N-[(2-methylpropoxy)carbonyl]alanyl-2-methylalanyl-2-amino-1,2,3,6,7,8-hexahydro-7,7-dimethyl-6,8-dioxo-2-pyrenecarbonyl-2-methylalanyl-2-methylalanyl-2-methylalanyl-2-methylalanyl-2-methylalanyl-7-amino-2,3,4,6,7,8-hexahydro-1,4-dimethyl-1H-cyclopenta[g]quinoxaline-7-carbonyl-2-methylalanyl-2-methylalanyl-, ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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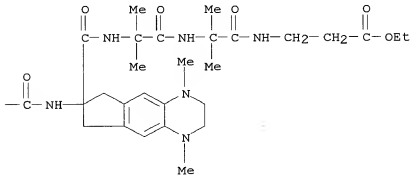
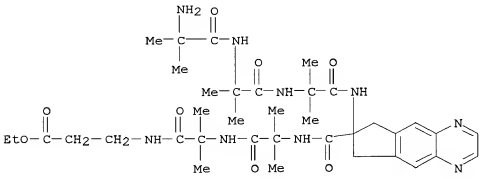


IT **253670-44-9**
RL: RCT (Reactant)
(reaction of in the synthesis of rigid 310-helical oligopeptides contg. redox cyclic .alpha.-amino acids for study of long-range electron transfer)

RN 253670-44-9 CAPLUS

CN .beta.-Alanine, 2-methylalanyl-2-methylalanyl-2-methylalanyl-7-amino-7,8-dihydro-6H-cyclopenta[g]quinoxaline-7-carbonyl-2-methylalanyl-2-methylalanyl-, ethyl ester (9CI) (CA INDEX NAME)



Searched by Barb O'Bryen, STIC 308-4291

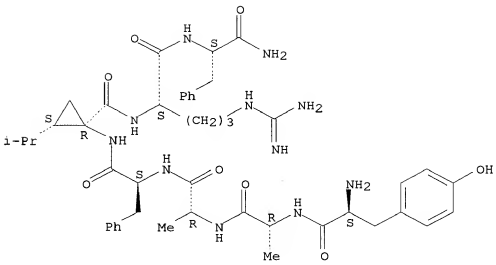
L5 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1997:707601 CAPLUS
DOCUMENT NUMBER: 128:18385
TITLE: Libraries of opiate and anti-opiate peptidomimetics containing 2,3-methanoleucine
AUTHOR(S): Burgess, Kevin; Li, Wen; Linthicum, D. Scott; Ni, Qing; Pledger, David; Rothman, Richard B.; Shitangkoon, Aroonsiri
CORPORATE SOURCE: Department of Chemistry, Texas AandM University, College Station, TX, 77843-3255, USA
SOURCE: Bioorg. Med. Chem. (1997), 5(9), 1867-1871
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A library of 96 peptides/peptidomimetics was prepd., in which half was based on the YGGFL-NH2 sequence, while the remainder were derivs. of a presumed anti-opiate peptide, YGGFLRF-NH2. Of the 48 compds. in each half of the library, 32 contained a stereoisomer of 2,3-methanoleucine substituted for Leu5. Binding of the YGGFL-NH2 derivs. to the .mu.-and .delta.-opioid receptors, and to the anti-.beta.-endorphin monoclonal antibody (clone 3E7), indicated any change at the Leu5 had little effect on the binding when compared with modifications to the YGGF-sequence. Conversely, cyclo-Leu residues did alter the binding of YGGFLRF-NH2 derivs. when substituted for Leu5. Of these 32 peptidomimetics, three derivs. of 2S,3S-cyclo-Leu had relatively low Ki values for binding to an NPFF receptor. Differences between the outcome of the screens were interpreted in terms of the position of the cyclo-Leu residue in the two sequences.

IT **185751-47-7 185751-51-3 185751-55-7**
**185751-59-1 185751-63-7 185751-67-1**
**185751-71-7 185751-75-1 199445-04-0**
**199445-05-1 199445-06-2 199445-07-3**
**199445-29-9 199445-31-3 199445-32-4**
**199445-33-5**
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); BIOL (Biological study)
(libraries of opiate and anti-opiate peptidomimetics contg. 2,3-methanoleucine)

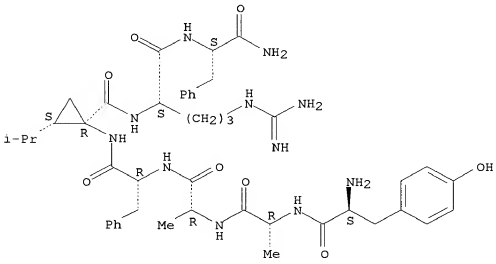
RN 185751-47-7 CAPLUS
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1R,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



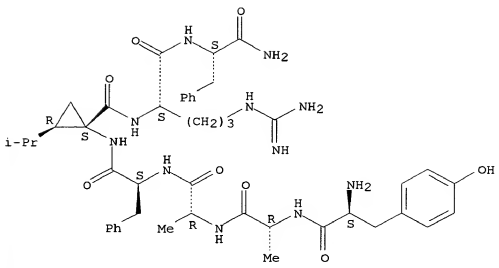
RN 185751-51-3 CAPLUS
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1R,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



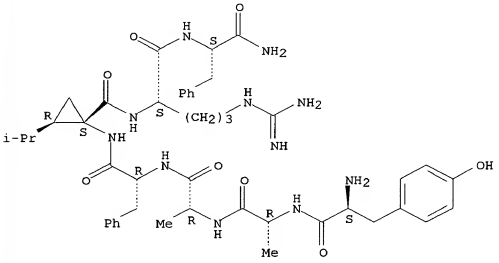
RN 185751-55-7 CAPLUS
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1S,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



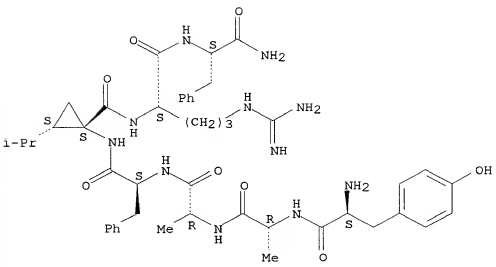
RN 185751-59-1 CAPLUS
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1S,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



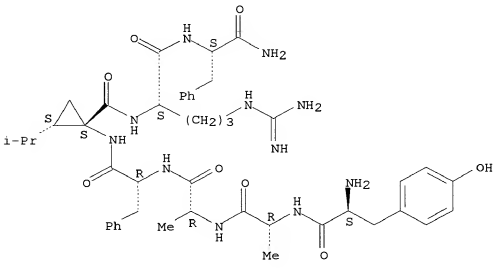
RN 185751-63-7 CAPLUS
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1S,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



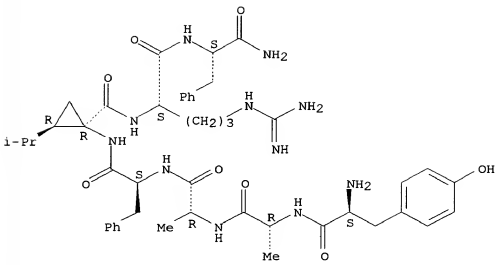
RN 185751-67-1 CAPLUS
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1S,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



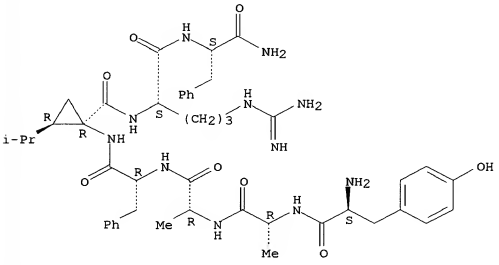
RN 185751-71-7 CAPLUS
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1R,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



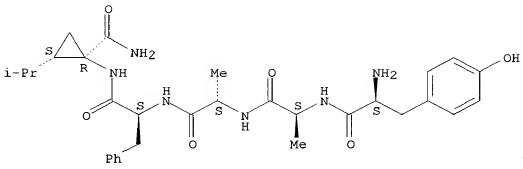
RN 185751-75-1 CAPLUS
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1R,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



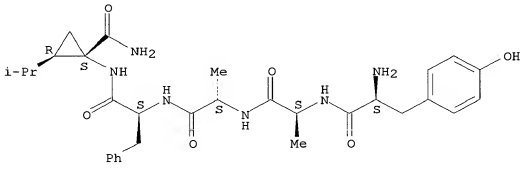
RN 199445-04-0 CAPLUS
CN Cyclopropanecarboxamide, L-tyrosyl-L-alanyl-L-alanyl-L-phenylalanyl-1-amino-2-(1-methylethyl)-, (1R,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 199445-05-1 CAPLUS
CN Cyclopropanecarboxamide, L-tyrosyl-L-alanyl-L-alanyl-L-phenylalanyl-1-amino-2-(1-methylethyl)-, (1S,2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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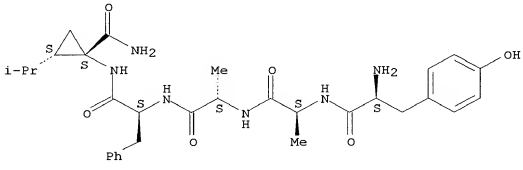
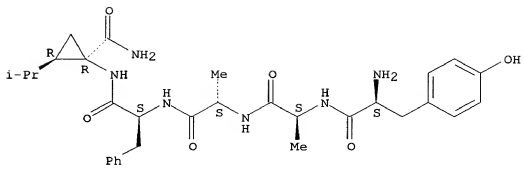
Absolute stereochemistry.



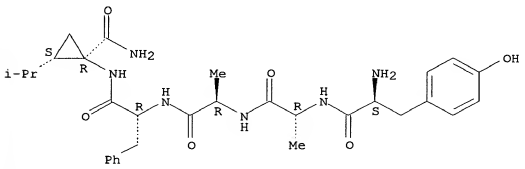
RN 199445-07-3 CAPLUS
CN Cyclopropanecarboxamide, L-tyrosyl-L-alanyl-L-alanyl-L-phenylalanyl-1-amino-2-(1-methylethyl)-, (1R,2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



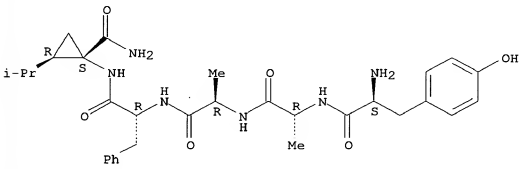
RN 199445-29-9 CAPLUS
CN Cyclopropanecarboxamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-1-amino-2-(1-methylethyl)-, (1R,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



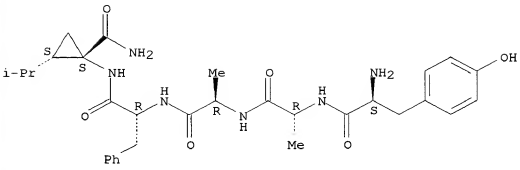
RN 199445-31-3 CAPLUS
CN Cyclopropanecarboxamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-1-amino-2-(1-methylethyl)-, (1S,2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 199445-32-4 CAPLUS
CN Cyclopropanecarboxamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-1-amino-2-(1-methylethyl)-, (1S,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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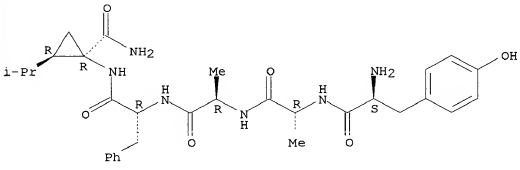
CN Cyclopropanecarboxamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-1-amino-2-(1-methylethyl)-, (1R,2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1997:646051 CAPLUS
DOCUMENT NUMBER: 127:307651
TITLE: Design and synthesis of novel nonpolar host peptides for the determination of the 310- and .alpha.-helix compatibilities of .alpha.-amino acid building blocks: an assessment of .alpha.,.alpha.-disubstituted glycines
AUTHOR(S): Obrecht, Daniel; Altorfer, Michael; Bohdal, Udo; Daly, John; Huber, Walter; Labhardt, Alexander; Lehmann, Christian; Muller, Klaus; Ruffieux, Ruth; Schonholzer, Peter; Spiegler, Clive; Zumbrunn, Cornelia
CORPORATE SOURCE: F. Hoffmann-La Roche AG, Pharma Research, Basel, CH-4070, Switz.
SOURCE: Biopolymers (1997), 42(5), 575-626
CODEN: BIPMAA; ISSN: 0006-3525
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The present work describes three novel nonpolar host peptide sequences that provide a ready assessment of the 310- and .alpha.-helix compatibilities of natural and unnatural amino acids at different positions of small- to medium-size peptides. The unpolar peptides contg. Ala, .alpha.-aminoisobutyric acid (Aib), and a C-terminal p-iodoanilide group were designed in such a way that the peptides could be rapidly assembled in a modular fashion, were highly sol. in solvent mixts. of triflouroethanol and H2 for CD and two-dimensional NMR analyses, and showed excellent crystallinitv suited for x-rav structure anal. To

validate this approach, 9-mer peptides, 12-mer peptides, and 10-mer peptides incorporating a series of optically pure cyclic and open-chain (R)- and (S)-.alpha.,.alpha.-disubstituted glycines were prepd. These amino acids are known to significantly modulate the conformations of small peptides. Based on x-ray structures, CD spectra recorded in acidic, neutral, and basic media and detailed 2D-NMR analyses, several interesting conformational observations were made. Esp. interesting results were obtained using the convex constraint CD anal. proposed by Fasman, which allowed the detn. of the relative content of 310- and .alpha.-helical conformations. These results were fully supported by the corresponding x-ray and 2D-NMR analyses. As a striking example, it was found that the (S)- and (R)-.beta.-tetralin derived amino acids show excellent .alpha.-helix stabilization, more pronounced than Aib and Ala. These novel ref. peptide sequences should help establish a scale for natural and unnatural amino acids concerning their intrinsic 310-and .alpha.-helix compatibilities at different positions of medium-sized peptides and thus improve the understanding of folding processes in peptides.

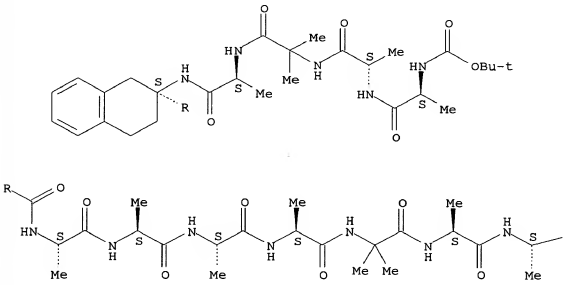
IT **197380-57-7P 197380-58-8P 197380-59-9P**
**197380-60-2P 197381-27-4P 197381-29-6P**
**197431-13-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(design and synthesis of novel nonpolar host peptides for the detn. of the 310- and .alpha.-helix compatibilities of disubstituted glycine building blocks)

RN 197380-57-7 CAPLUS

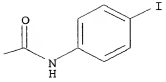
CN L-Alaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-(2S)-2-amino-1,2,3,4-tetrahydro-2-naphthalenecarbonyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A



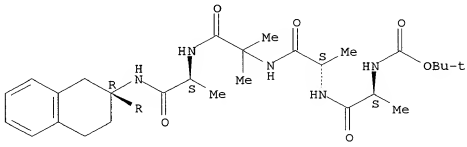
PAGE 1-B

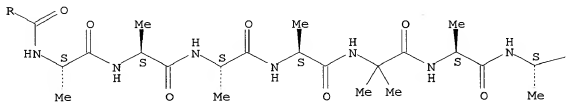


RN 197380-58-8 CAPLUS
CN L-Alaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-(2R)-2-amino-1,2,3,4-tetrahydro-2-naphthalenecarbonyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

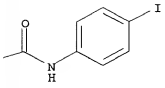
Absolute stereochemistry.

PAGE 1-A





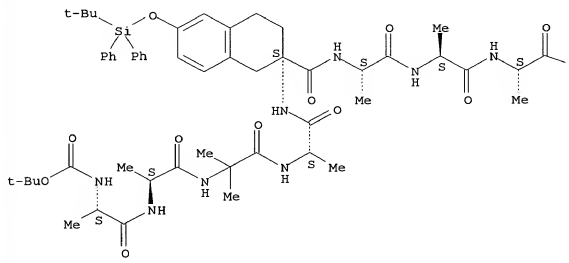
PAGE 1-B



RN 197380-59-9 CAPLUS
CN L-Alaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-(2S)-2-amino-6-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-1,2,3,4-tetrahydro-2-naphthalenecarbonyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A



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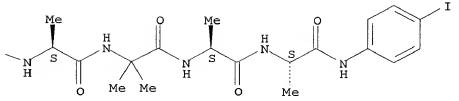
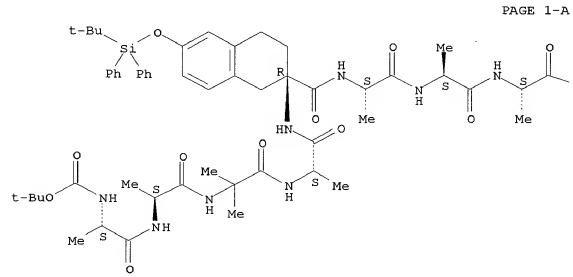


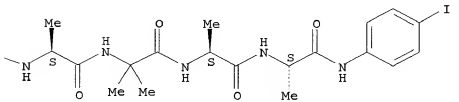
RN 197380-60-2 CAPLUS
CN L-Alaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-(2R)-2-amino-6-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-1,2,3,4-tetrahydro-2-naphthalenecarbonyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A



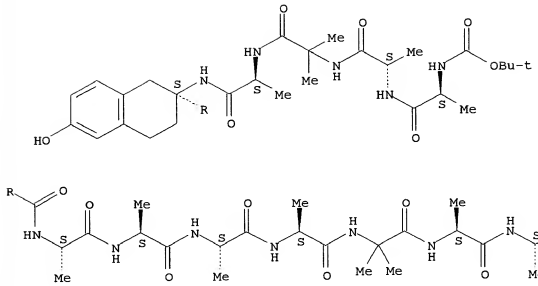
PAGE 1-B



RN 197381-27-4 CAPLUS
CN L-Alaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-(2S)-2-amino-1,2,3,4-tetrahydro-6-hydroxy-2-naphthalenecarbonyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A



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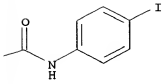
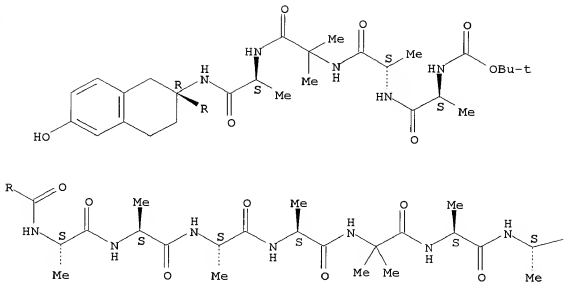


RN 197381-29-6 CAPLUS
CN L-Alaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-(2R)-2-amino-1,2,3,4-tetrahydro-6-hydroxy-2-naphthalenecarbonyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A



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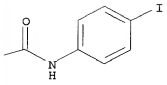
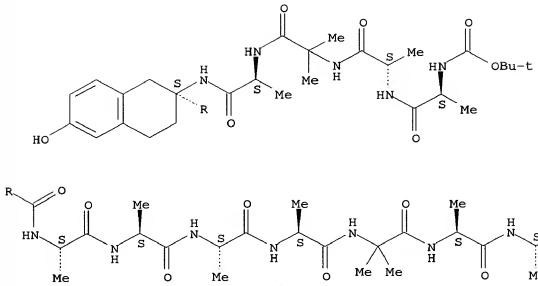


RN 197431-13-3 CAPLUS
CN L-Alaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-(2S)-2-amino-1,2,3,4-tetrahydro-6-hydroxy-2-naphthalenecarbonyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)-, monohydrate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A



PAGE 1-B

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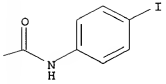


L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2000 ACS

| | |
|---|---|
| ACCESSION NUMBER: | 1996:741618 CAPLUS |
| DOCUMENT NUMBER: | 126:89768 |
| TITLE: | A small library of peptidomimetics to systematically vary and test the effects of x1 constraints |
| AUTHOR(S): | Burgess, Kevin; Godbout, Claude; Li, Wen; Payza, Kemal |
| CORPORATE SOURCE: | Department Chemistry, Texas A & M University, College Station, TX, 77843-3255, USA |
| SOURCE: | Bioorg. Med. Chem. Lett. (1996), 6(22), 2761-2764 CODEN: BMCLE8; ISSN: 0960-894X |
| PUBLISHER: | Elsevier |
| DOCUMENT TYPE: | Journal |

Searched by Barb O'Bryen, STIC 308-4291

LANGUAGE: English

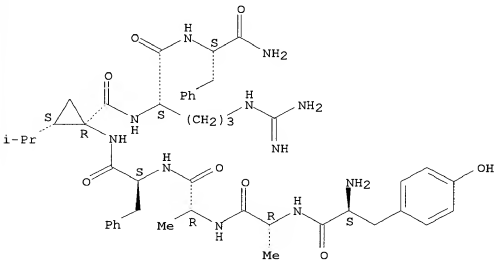
AB A library of 47 peptidomimetics of H-Tyr-Gly-Gly-Phe-Leu-Arg-Phe-NH2 was prepd. wherein 32 of these contained one of the four different isomers of the conformationally constrained 2,3-methanoleucine for Leu5. This library was tested for binding the neuropeptide FF receptor where neuropeptide FF is H-Phe-Leu-Phe-Gln-Pro-Gln-Arg-Phe-NH2, an anti-opiate peptide. This study illustrates how conformational constraints can be systematically varied in a library format to det. the best conformational restrictions for the desired activity.

IT **185751-47-7P 185751-51-3P 185751-55-7P**
**185751-59-1P 185751-63-7P 185751-67-1P**
**185751-71-7P 185751-75-1P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of a peptidomimetic library contg. conformationally constrained methanoleucine)

RN 185751-47-7 CAPLUS

CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1R,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

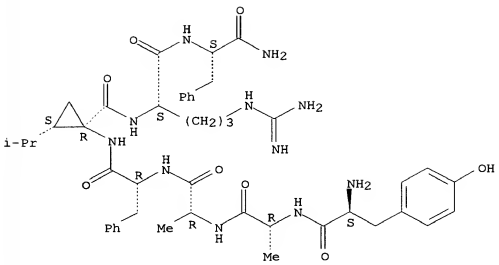
Absolute stereochemistry.



RN 185751-51-3 CAPLUS

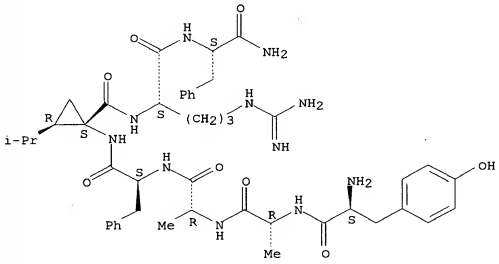
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1R,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



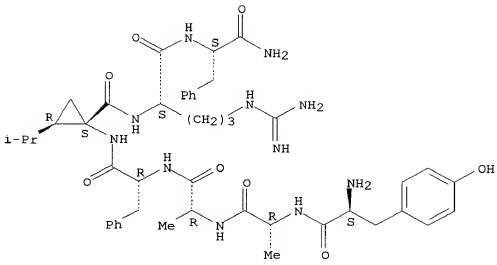
RN 185751-55-7 CAPLUS
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1S,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



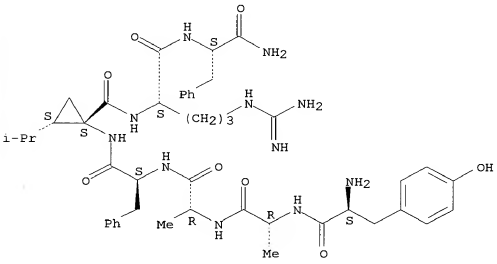
RN 185751-59-1 CAPLUS
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1S,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



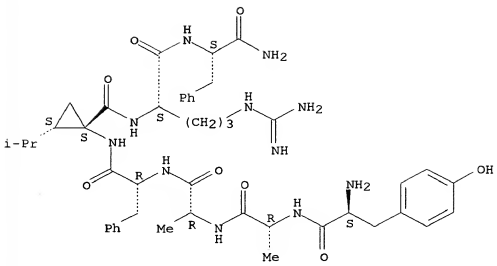
RN 185751-63-7 CAPLUS
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1S,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



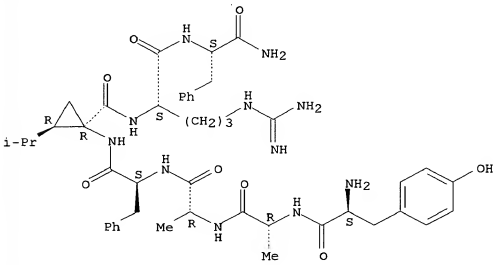
RN 185751-67-1 CAPLUS
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1S,2S)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



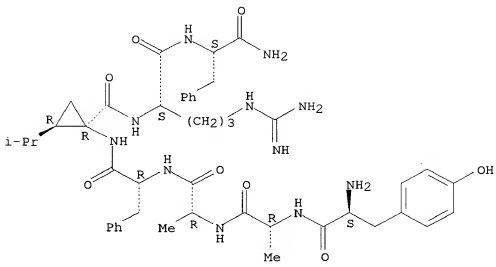
RN 185751-71-7 CAPLUS
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-L-phenylalanyl-(1R,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 185751-75-1 CAPLUS
CN L-Phenylalaninamide, L-tyrosyl-D-alanyl-D-alanyl-D-phenylalanyl-(1R,2R)-1-amino-2-(1-methylethyl)cyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1995:846974 CAPLUS
DOCUMENT NUMBER: 123:257365
TITLE: .alpha.-Helical versus 310-Helical Conformation of Alanine-Based Peptides in Aqueous Solution: An Electron Spin Resonance Investigation
AUTHOR(S): Smythe, Mark L.; Nakaie, Clovis R.; Marshall, Garland R.
CORPORATE SOURCE: School of Medicine, Washington University, St. Louis, MO, 63110, USA
SOURCE: J. Am. Chem. Soc. (1995), 117(42), 10555-62
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:257365

AB Due to the difficulties in exptl. differentiating between the .alpha.- and 310-helical conformations in soln., isolated helical peptides were assumed to be in the .alpha.-helical conformation. However, recent ESR studies have suggested that such peptides, in particular short alanine-based peptides, are 310-helical (Miick, S. M.; et al. 1992). This result prompted the authors to further investigate the helical conformations of alanine-based peptides in soln. using ESR. Unlike previous investigations with a flexible link connecting the spin-label to the peptide backbone, the authors used a conformationally constrained spin-label (4-amino-4-carboxy-2,2,6,6-tetramethylpiperidine-1-oxyl, Toac) that is rigidly attached to the peptide backbone. From a combination of mol. modeling and ESR spectroscopy investigations, it was concluded that these alanine-based peptides exist primarily in the .alpha.-helical conformation, and not the 310-form as previously suggested for an analogous set of peptides in aq. environments. This discrepancy is thought to be due to the differences in flexibility of the spin-labels employed. The conformationally constrained spin-label Toac used in this study should accurately reflect the backbone conformation. Free energy surfaces, or potentials of mean force, for the conformational transition of the spin-label used in previous studies (Miick S. M.; et al. 1992) suggest that this spin-label is too flexible to accurately distinguish between the .alpha.- and 310-helical conformations.

IT **169134-77-4P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(.alpha.-helical vs. 310-helical conformation of alanine-based peptides

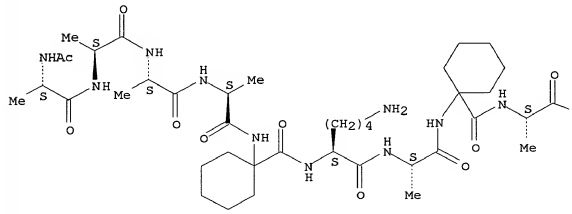
in aq. soln. by ESR of spin-labeled derivs.)

RN 169134-77-4 CAPLUS

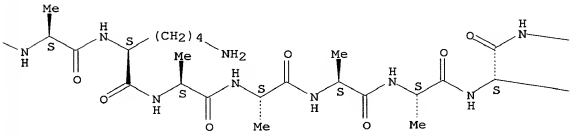
CN L-Alaninamide, N-acetyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-1-aminocyclohexanecarbonyl-L-lysyl-L-alanyl-1-aminocyclohexanecarbonyl-L-alanyl-L-alanyl-L-lysyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-L-lysyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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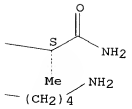
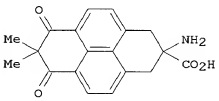


L5 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1995:380710 CAPLUS
DOCUMENT NUMBER: 122:161358
TITLE: Helical Stability of de Novo Designed .alpha.-Aminoisobutyric Acid-Rich Peptides at High Temperatures
AUTHOR(S): Augspurger, J. D.; Bindra, V. A.; Scheraga, H. A.; Kuki, A.
CORPORATE SOURCE: Baker Laboratory of Chemistry, Cornell University, Ithaca, NY, 14853-1301, USA
SOURCE: Biochemistry (1995), 34(8), 2566-76
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB 1- And 2-dimensional NMR spectroscopy is used to det. the helical stability of two Aib-rich peptides, Me2CHCH2O2C-(Aib)3-DkNap-Leu-Aib-Ala-(Aib)2-NHCH2CH2OMe (DkNap = phenylenedione-based amino acid I) (Dk4[7/9]) and Ac-(Aib)2-Nap-(Aib)2-Phe-(Aib)2-NHMe [Nap = .beta.-(1-naphthyl)-L-alanine] (Nap3Phe6[6/8]), where the bracket notation indicates the no. of Aib-class residues/total no. of residues. 2D ROESY expts., carried out previously on Nap3Phe6[6/8] in DMSO (Basu, G., & Kuki, A. 1993), showed that this compd. adopts the 310-helical conformation at 20 .degree.C. The first step in the present work is to apply this technique to the peptide Dk4[7/9], demonstrating that it likewise adopts the 310-helical conformation in chloroform at 20.degree.. The amide proton shifts of Nap3Phe6[6/8] in DMSO and Dk4[7/9] in C2D2Cl4 were then monitored by 1-dimensional NMR over a large temp. range, up to 150 and 120.degree., resp. The nonamer Dk4[7/9] exhibits no evidence of any conformational or unfolding transition as the temp. is raised. The nearly temp. independent amide proton chem. shifts of this nonamer are an indication of retention of the intrahelical hydrogen bonding, which was then verified directly by solvent perturbation with DMSO at 120.degree.. The resulting

hydrogen-bonding pattern confirms that Dk4[7/9] retains its 310-helical conformation in C2D2Cl4 over the entire temp. range. This conformational quietness is exploited to examine the intrinsic temp. dependence of free vs. intrahelically hydrogen bonded amide proton shifts within the same peptide structure. It is also shown that Nap3Phe6[6/8] retains its 310-helical conformation over the entire temp. range in the stronger hydrogen-bonding solvent DMSO. The extreme thermal stability of these octameric and nonameric Aib-rich peptides in both solvents is contrasted with that of much longer alanine-rich peptides in water.

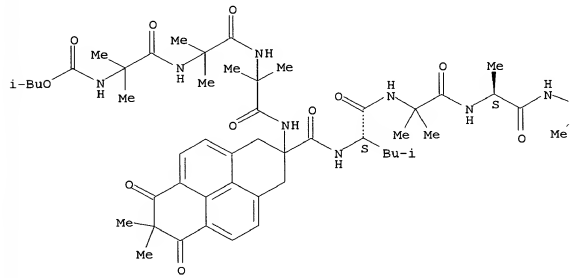
IT **157662-09-4**
RL: PRP (Properties)
(helical stability of de novo designed .alpha.-aminoisobutyric acid-rich peptides at high temps.)

RN 157662-09-4 CAPLUS

CN Alaninamide, 2-methyl-N-[(2-methylpropoxy)carbonyl]alanyl-2-methylalanyl-2-methylalanyl-1,2,3,6,7,8-hexahydro-7,7-dimethyl-6,8-dioxo-2-amino-2-pyrenecarbonyl-L-leucyl-2-methylalanyl-L-alanyl-2-methylalanyl-N-(2-methoxyethyl)-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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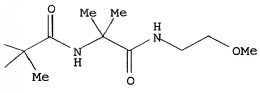
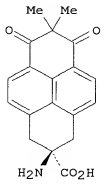


L5 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2000 ACS
Searched by Barb O'Bryen, STIC 308-4291

ACCESSION NUMBER: 1995:285530 CAPLUS
DOCUMENT NUMBER: 122:161342
TITLE: Conformational preferences of oligopeptides rich in .alpha.-aminoisobutyric acid. III. Design, synthesis and hydrogen bonding in 310-helixes
AUTHOR(S): Bindra, Vandana A.; Kuki, Atsuo
CORPORATE SOURCE: Dep. Chem. Baker Lab., Cornell Univ., Ithaca, NY, USA
SOURCE: Int. J. Pept. Protein Res. (1994), 44(6), 539-48
CODEN: IJPPC3; ISSN: 0367-8377
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

DkNap =

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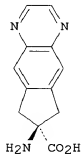



AB Two sterically constrained peptides, iBoc-(Aib)3-DkNap-Leu-X-Ala-Aib-Aib-Fl (I; Aib = .alpha.-aminoisobutyric acid; Fl = NHCH2CH2OMe; iBoc = Me2CHCH2O2C; X = Aib, Qx), contg. Aib and Aib-class amino acids in conjunction with selected mono-.alpha.-alkyl amino acids were synthesized by an optimized procedure. The use of Aib-class amino acids DkNap and Qx gives rise to the same overwhelmingly 310-helical backbone conformation as that provided by simpler Aib-rich peptides and homopeptides. The synthetic .alpha.,.alpha.-dialkylamino acids DkNap and Qx are arom. homologues of the known alicyclic variants of Aib, the Ac5c and Ac6c amino acids. Two new org. solubilizing groups for peptides, iBoc and Fl, are introduced. The 1H NMR analyses of I demonstrate the unambiguous 210-helical hydrogen bonding pattern of these peptides, confirming the design objective of these sequence patterns contg. greater than 50% Aib and Aib-class compn.

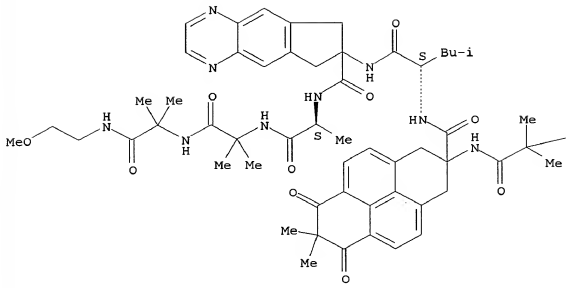
IT **157662-08-3P 157662-09-4P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(design, synthesis, and hydrogen bonding in 310-helical .alpha.-aminoisobutyric acid-contg. peptides and analogs)

RN 157662-08-3 CAPLUS

CN Alaninamide, 2-methyl-N-[(2-methylpropoxy)carbonyl]alanyl-2-methylalanyl-2-methylalanyl-1,2,3,6,7,8-hexahydro-7,7-dimethyl-6,8-dioxo-2-amino-2-pyrenecarbonyl-L-leucyl-7,8-dihydro-7-amino-6H-cyclopenta[g]quinoxaline-7-carbonyl-L-alanyl-2-methylalanyl-N-(2-methoxyethyl)-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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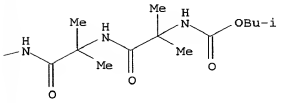
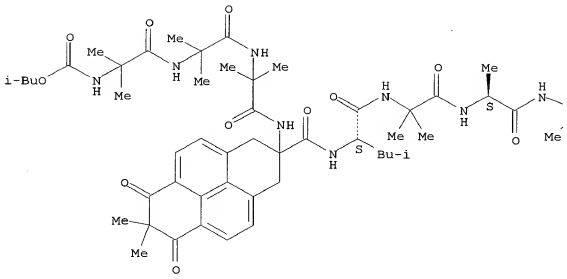


RN 157662-09-4 CAPLUS
CN Alaninamide, 2-methyl-N-[(2-methylpropoxy)carbonyl]alanyl-2-methylalanyl-2-methylalanyl-1,2,3,6,7,8-hexahydro-7,7-dimethyl-6,8-dioxo-2-amino-2-pyrenecarbonyl-L-leucyl-2-methylalanyl-L-alanyl-2-methylalanyl-N-(2-methoxyethyl)-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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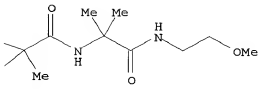

L5 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2000 ACS

| | |
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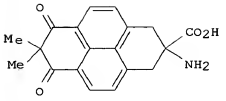
| ACCESSION NUMBER: | 1994:580159 CAPLUS |
| DOCUMENT NUMBER: | 121:180159 |
| TITLE: | Photoinduced electron transfer and long-lived charge separation in rigid peptide architectures |
| AUTHOR(S): | Anglos, Demetrios; Bindra, Vandana; Kuki, Atsuo |
| CORPORATE SOURCE: | Dep. Chem., Cornell Univ., Ithaca, NY, 14853-1301, USA |
| SOURCE: | J. Chem. Soc., Chem. Commun. (1994), (2), 213-15<br>CODEN: JCCCAT; ISSN: 0022-4936 |
| DOCUMENT TYPE: | Journal |
| LANGUAGE: | English |
| GI | |

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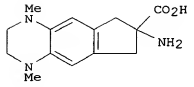



II

AB Phenylenedione-based amino acid I (DkNap) and tetrahydroquinoxaline-based amino acid II (ThQx) were used to construct two novel architectures, cyclo(DkNap-ThQx) and helical .alpha.-aminoisobutyric acid (Aib)-rich nonapeptide Me2CHCH2O2C-(Aib)3-DkNap-Leu-ThQx-Ala-(Aib)2-NHCH2CH2OMe, providing a rigid structural framework for the study of intramol., photoinduced electron transfer between the two custom-designed donor-acceptor redox .alpha.-amino acids.

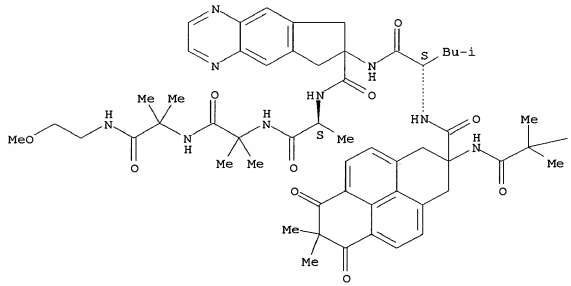
IT **157662-08-3 157662-09-4**
RL: PRP (Properties)
(conformation of, by NMR)

RN 157662-08-3 CAPLUS

CN Alaninamide, 2-methyl-N-[(2-methylpropoxy)carbonyl]alanyl-2-methylalanyl-2-methylalanyl-1,2,3,6,7,8-hexahydro-7,7-dimethyl-6,8-dioxo-2-amino-2-pyrenecarbonyl-L-leucyl-7,8-dihydro-7-amino-6H-cyclopenta[g]quinoxaline-7-carbonyl-L-alanyl-2-methylalanyl-N-(2-methoxyethyl)-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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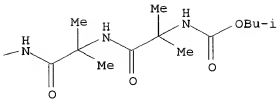
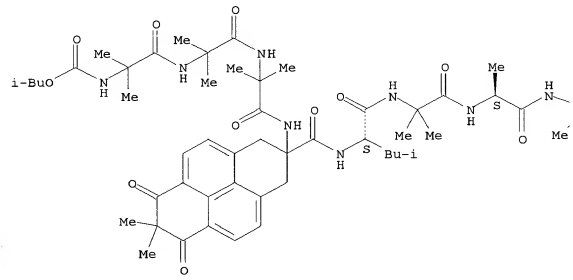


RN 157662-09-4 CAPLUS
CN Alaninamide, 2-methyl-N-[(2-methylpropoxy)carbonyl]alanyl-2-methylalanyl-2-methylalanyl-1,2,3,6,7,8-hexahydro-7,7-dimethyl-6,8-dioxo-2-amino-2-pyrenecarbonyl-L-leucyl-2-methylalanyl-L-alanyl-2-methylalanyl-N-(2-methoxyethyl)-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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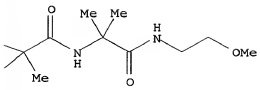
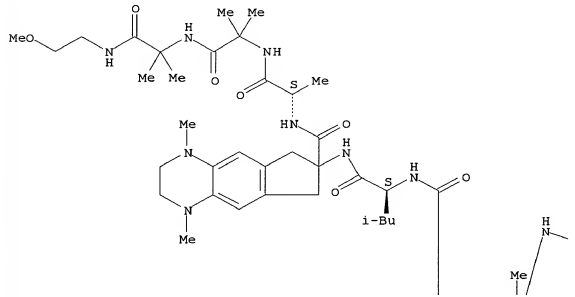


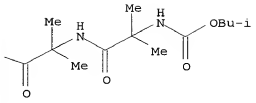
IT **157662-07-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., conformation, and intramol. photoinduced electron transfer of)
RN 157662-07-2 CAPLUS
CN Alaninamide, 2-methyl-N-[(2-methylpropoxy)carbonyl]alanyl-2-methylalanyl-2-methylalanyl-1,2,3,6,7,8-hexahydro-7,7-dimethyl-6,8-dioxo-2-amino-2-pyrenecarbonyl-L-leucyl-2,3,4,6,7,8-hexahydro-1,4-dimethyl-7-amino-1H-cyclopenta[g]quinoxaline-7-carbonyl-L-alanyl-2-methylalanyl-N-(2-methoxyethyl)-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

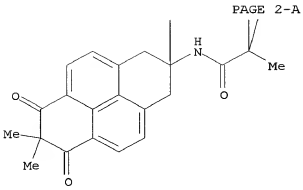
PAGE 1-A



PAGE 1-B



PAGE 2-A



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FILE COVERS 1907-1966
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This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, and patent assignees are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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